Determining Molecular Formulas.

May 2, 2011.

To determine a molecular formula you must have at least two pieces of information. You must know the molar mass of the compound and either the empirical formula or you need the percentage composition.

To calculate the subscripts we use a procedure similar to that used to determine empirical formula.

Start by assuming there is one mole of the compound. If you have the empirical formula the find the molar mass of it. Divide the molar mass of the compound by the molar mass of the empirical formula to get a factor we must multiply the empirical formula by.

Example #1: What is the molecular formula of a compound that has a molar mass of 120.12 g/mol and an empirical formula of CH_2O?

$$M_{CH_2O} = 12.01\ g/mol + 2(1.01\ g/mol) + 16.00\ g/mol$$

$$= 30.03\ g/mol$$

$$f = \frac{M_{compound}}{M_{empirical}} = \frac{120.12\ \cancel{g/mol}}{30.03\ \cancel{g/mol}} = 4.$$

∴ the molecular formula is $4(CH_2O)$ or $C_4H_8O_4$

If you have the percentage composition assume there is one mole of the compound and then use the percentage composition to determine the mass of each element present. Convert the mass of each element into a number of moles. The ratio of the moles of each element are the subscripts of the molecular formula.

Example #2: A compound has a molar mass of 75.08 g/mol. Analysis shows that it is 32.0% C, 6.70% hydrogen, 42.6% oxygen and 18.7% nitrogen. What is the molecular formula?

Solution

Assume there is mole of the compound.

$m_C = 32.0\% \times 75.08\,g = 24.02\,g$

↑ is mass of one mole of compound

$m_H = 6.7\% \times 75.08\,g = 5.03\,g$

$m_O = 42.6\% \times 75.08\,g = 31.98\,g$

$m_N = 18.7\% \times 75.08\,g = 14.04\,g.$

$n_C = 24.02\,g \times \frac{1\,mol}{12.01\,g} = 2\ mol$

$n_H = 5.03\,g \times \frac{1\,mol}{1.01\,g} = 5\ mol$

$n_O = 31.98\,g \times \frac{1\,mol}{16.00\,g} = 2\ mol$

$n_N = 14.04\,g \times \frac{1\,mol}{14.01\,g} = 1\ mol$

$\therefore$ the molecular formula is $C_2H_5O_2N$.